## Transmittal Summary Document ORD Manuscript Review

#### 1. Manuscript Title:

Use of Nontargeted PFAS to Develop a Legacy PFAS Fingerprint in New Jersey

**Authors:** John W. Washington<sup>1\*</sup>, Charlita G. Rosal<sup>1</sup>, James P. McCord<sup>2</sup>, Mark J. Strynar<sup>2</sup>, Andrew B. Lindstrom<sup>2</sup>, Erica L. Bergman<sup>3</sup>, Sandra M. Goodrow<sup>3</sup>, Haile K. Tadesse<sup>2</sup>, Andrew N. Pilant<sup>2</sup>, Benjamin J. Washington<sup>4</sup>, Mary J. Davis<sup>1</sup>, Brittany G. Stuart<sup>5</sup>, Thomas M. Jenkins<sup>6</sup>

Affiliations: <sup>1</sup>USEPA, Office Research and Development, Athens, GA. <sup>2</sup>USEPA, Office Research and Development, Research Triangle Park, NC. <sup>3</sup>NJDEP, Division of Science and Research, Trenton, NJ. <sup>4</sup>USEPA, Office Research and Development, Washington, DC. <sup>5</sup>USEPA, Office of Research and Development, Cincinnati, OH. <sup>6</sup>Senior Environmental Employment Program (USEPA/ORD), Athens, GA.

#### 2. Background/Overview:

New Jersey Department of Environmental Protection (NJDEP) requested ORD's assistance to investigate legacy PFAS distribution in NJ, including two potential PFAS sources. NJDEP collected soil, vegetation and water samples from transects and from across much of the state, delivering soil/veg samples to Athens and water to RTP.

In this manuscript, we report on soil PFAS in New Jersey, **not US water**. In soil, we identified ten new PFAS compounds, chlor-perfluoro-polyether-carboxylates (ClPFPECAs), using nontargeted analyses and semiquantitated the concentrations of these compounds. We contoured these ClPFPECA values on a map, forming a pattern focusing on one of the potential sources identified by NJDEP.

We used the CIPFPECA data, and PFAS reaction stoichiometry, to develop a fingerprint of legacy PFAS. When this legacy fingerprint was contoured on a map, it formed a pattern focusing on both potential sources identified by NJDEP.

#### 3. Relevancy to program office/regional research needs/priorities:

The data and information reported here suggest that fingerprinting of PFAS may be possible in certain situations to support risk managers in identifying sources of specific PFAS.

4. Name(s) of program/regional office coauthors or reviewer(s) of earlier drafts, if any No program or regional coauthors or reviewers. Staff from NJ DEP are included as coauthors. Draft manuscript has been shared for awareness with R2 POC for the NJ collaboration.

#### 5. Major observations and results:

Collectively, our results: (i) identify ten novel PFAS, ClPFPECAs, not previously detected in the environment, including congeners with no previous reports, so far as we know; (ii) Ex. 5 Deliberative Process (DP)

### Ex. 5 Deliberative Process (DP)

**Ex. 5 Deliberative Process (DP)**y; (iv) indicate the source of these CIPFPECAs in New Jersey dominantly are from Solvay; (v) were used to fingerprint historical sources of legacy long-chain PFCAs C11 and C13 being from Solvay, and C10 and C12 from the Chemours facility; and (vi) document discernable signals of these legacy PFCAs across an expansive breadth of south Jersey persisting today.

# Ex. 5 Deliberative Process (DP)

#### 7. Findings advancing existing scientific knowledge:

Advances in scientific knowledge include: (i) identification/elucidation of ten new PFAS congeners, potentially with isomers, in the environment; (ii) development of methods to detect these compounds on conventional LC/MS/MS; (iii) document sorting of PFAS in atmospheric plumes by molecular mass, perhaps for the first time; (iv) document considerable atmospheric transport distances of PFAS having very low vapor pressures (i.e., chemically non-gaseous PFAS), contrary to expectations of many chemists (e.g., me); (v) reporting of semiquantitative concentrations of nontargeted analytes for the first time in the peer-reviewed literature so far as I know (I had reported semi-quantitated values for targeted compounds in the past but not nontargeted); (vi) perhaps reports one of the first fingerprints of legacy compounds in a complex contaminant setting – there's lots of literature noise about fingerprinting, but I have seen no real-world examples that aren't isolated sites in generally pristine surroundings or unique compounds.

#### 8. Publication information (journal, book) and estimated timelines:

Optimistically, I hope to have this thru clearance by the end of November. When clearance is complete, I plan to submit to the journal Science. Realistically, I understand the strong chance of rejection by Science at which time I would rewrite for format and submit to ES&T.